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Local versus homogenized field yield criterion for failure in amorphous polymers

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ABSTRACT

Despite a large number of experiments and simulations, there is inconsistency between homogenized and local field criteria for yielding in glassy polymers. Although atomistic simulations can attain local field values of stress and strain at failure, experiments provide yield conditions in terms of homogenized field values. Simulations at the micromechanical level are implemented here where the local and homogenized yield conditions can be calculated simultaneously. We present a phase field damage mode (PFDM) informed directly from atomistic simulations to analyze the response of structures comparable in length and time scales to experiments. We calculate the stress and strain invariants at yield with homogenized and local fields at the same time. Furthermore, our results show that homogenized yield criteria do not agree with criteria obtained locally and therefore cannot be used directly to determine yield conditions in local fields. On the other hand, the yield surfaces based on the local strain invariants have good agreement with local theories of failure that rely on dehomogenization like the micro mechanical enhancement method. We show how the PFDM developed here can be used to reduce the uncertainty on the definition of the critical strains in these models.